

Optimal Control for Electron Shuttling

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(Dated: August 15, 2012)

In this paper we apply optimal control technique to derive the control fields that transfer electron from one end of a chain of donors or quantum dots to the other. We formulate it as an optimal steering problem, and then derive the dynamics of the optimal control. A numerical algorithm is developed to efficiently generate control pulses. We apply this technique to transfer an electron between sites of a triple quantum dot and an ionized chain of phosphorus dopants in silicon, in which we show that a 500 G magnetic field will transfer the electron and two of the four hyperfine states of the electron-nuclear spin pair.

I. PHYSICAL BACKGROUNDS

The benefits of implementing a quantum computer in silicon [1], namely the ability to exploit the techniques of the semiconductor industry and long spin coherence times, has been offset with challenges including the coupling of qubits. One mechanism for exchanging quantum information between qubits is electron shuttling, in which spin or charge qubits are literally moved between local sites [2]. For dopant spin qubits in silicon [3], electron shuttling has been proposed using voltage gates and pulses designed analogously to the STIRAP procedure [4]; this procedure is referred to as coherent tunneling by adiabatic passage (CTAP) [5–7]. Similar mechanisms have been suggested [8] for quantum dots in silicon, which have also been proposed as qubits [9–14]. CTAP and other adiabatic procedures avoid populating undesired sites at any point during the transfer, thereby eliminating issues of decoherence associated with a specific site. However, if the source of decoherence is not site-specific or is controllable by alternative means, it may be useful to approach the state transfer problem for silicon qubits using optimal control theory instead. Optimal controls which minimize transfer time or (as will be explored here) minimize pulse fluence have been shown to minimize decoherence due to additive and multiplicative white noise, respectively [15, 16]. Additionally, for qubits such as charge qubits in which site-specific decoherence is not the main problem, we can use optimal controls in order to minimize the energy required for gate operations.

In this paper we will investigate the shuttling of electrons between the ends of a qubit chain using optimal control theory. Depending on whether the chain represents dopant spin qubits [5, 7] or lateral quantum dots [8], the control fields will affect the tunnel couplings between dopants or the on-site energy of a quantum dot, respectively. The task is to design some appropriate control fields to transport the electron to the end of the qubit chain. During this process, quantum information can be passed through along the array so as to realize the desired quantum information processing in the solid-state

quantum bits.

This problem can be formulated as an optimal steering problem in control theory. The state space consists of all the density matrices, *i.e.*, Hermitian matrices with unit trace. The system dynamics is governed by Liouville-von Neumann equation. The Hamiltonian usually contains a drift term, which is a fixed term determined by the physical nature of the system, and several control terms that can be altered externally as a function of time. The objective of steering is to find control fields to transfer the system from an initial state to a final state at a finite terminal time. This is also known as constructive controllability problem [17].

One way to solve this problem is to impose a cost function, which may encode minimum energy, shortest time, or tracking error penalty. We can then employ standard optimal control technique such as Pontryagin Maximum Principle [18] to derive optimality conditions for optimal control fields. These conditions result in a two-point boundary-value problem, which is often difficult to solve numerically.

In the current paper we derive the underlying dynamics that governs the time evolution of optimal control. We take an intuitive approach, which yields the same results as from sophisticated Lie-Poisson reduction theorem [19]. For a given initial condition for this dynamics, it completely determines the time evolution trajectories of controls. Hence, to solve for control fields that achieve the desired state transfer, we just need to find an appropriate initial condition. It thus becomes an optimization problem on finite dimensional real space.

To solve the Liouville-von Neumann equation numerically, we divide the total time duration into a number of small steps and then use piecewise constant functions to approximate time-varying control fields. The fidelity of the achieved states thus depends on all of the piecewise constant control values, which consequently are dependent on the initial conditions of the dynamics discussed above. Using the chain rule, we can obtain the gradient of the fidelity with respect to the initial condition in closed-form solution. With this approach we can now

implement mature gradient type of algorithms to solve for control fields that accomplish the steering task.

To exemplify this approach, we investigate the electron shuttling problem for three-donor systems in this paper. Our control algorithm derivation can be readily extended to both systems with more donors and to alternative objective functions such as minimizing spin decoherence during spatial transfer. We demonstrate the efficacy of our control algorithm by applying it to two physical systems in Refs. [5] and [8] and then generating the control functions to realize the electron shuttling.

II. MATHEMATICAL BACKGROUND AND FORMULATION

In this section we introduce some necessary mathematical background and a general description of the electron shuttling problem.

We consider physical devices with three qubits. This type of system has been previously studied in Refs. [5, 7, 8]. The system Hamiltonian is defined on Lie algebra $\mathfrak{su}(3)$, *i.e.*, all the 3×3 skew-Hermitian matrices. Define a basis for $\mathfrak{su}(3)$ as

$$\begin{aligned} X_1 &= \begin{bmatrix} 0 & i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, & X_2 &= \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & i \\ 0 & i & 0 \end{bmatrix}, \\ X_3 &= \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{bmatrix}, & X_4 &= \begin{bmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \\ X_5 &= \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{bmatrix}, & X_6 &= \begin{bmatrix} 0 & 0 & i \\ 0 & 0 & 0 \\ i & 0 & 0 \end{bmatrix}, \\ X_7 &= \begin{bmatrix} i & 0 & 0 \\ 0 & -i & 0 \\ 0 & 0 & 0 \end{bmatrix}, & X_8 &= \frac{1}{\sqrt{3}} \begin{bmatrix} i & 0 & 0 \\ 0 & i & 0 \\ 0 & 0 & -2i \end{bmatrix}. \end{aligned} \quad (1)$$

Define the numbers $C_{ij}^k \in \mathbb{C}$ such that

$$[X_i, X_j] = \sum_{k=1}^K C_{ij}^k X_k, \quad (2)$$

where K is the dimension of the Lie algebra and $K = 8$ for $\mathfrak{su}(3)$. These numbers are the *structure constants* of the Lie algebra $\mathfrak{su}(3)$ with respect to the basis $\{X_k\}_{k=1}^K$. Note that the structure constants are antisymmetric in all the indices, *i.e.*,

$$C_{ij}^k = -C_{ji}^k = -C_{kj}^i = -C_{ik}^j, \quad (3)$$

for all $i, j, k \in \{1, \dots, K\}$. Up to antisymmetry, the nonzero structure constants are

$$\begin{aligned} C_{12}^3 &= -1, & C_{14}^7 &= -2, & C_{15}^6 &= 1, \\ C_{24}^6 &= -1, & C_{25}^7 &= 1, & C_{25}^8 &= -\sqrt{3}, \\ C_{34}^5 &= 1, & C_{36}^7 &= 1, & C_{36}^8 &= \sqrt{3}. \end{aligned} \quad (4)$$

We also use the usual matrix inner product

$$\langle X, Y \rangle = \text{Tr}(XY^\dagger). \quad (5)$$

The dynamics of donor system is determined by the Liouville-von Neumann equation:

$$\dot{\rho} = -[iH, \rho]. \quad (6)$$

The Hamiltonian H of three donors system can be written in a general form as

$$iH = iH_0 + \sum_{l=1}^p u_l X_l = \sum_{l=p+1}^K a_l X_l + \sum_{l=1}^p u_l X_l, \quad (7)$$

where H_0 is the drift term, and u_l are control fields. The implementation of the electron shuttling from one end of the donor chain to the other amounts to design control functions u_l to transfer the density matrix ρ from the initial state

$$\rho_0 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \quad (8)$$

at time $t = 0$ to the final state

$$\rho_T = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad (9)$$

at time $t = T$.

III. OPTIMAL CONTROL AND NUMERICAL ALGORITHM

To solve the state transfer problem (6)-(9), we impose a cost function to formulate it as an optimal control problem, and then use optimal control theory to derive the optimality conditions. Based on these conditions, we develop a numerical algorithm to solve control fields efficiently.

A. Optimal control formulation

For the steering problem (6)-(9), in addition to realize the desired state transfer, we seek the control fields that minimize the following energy type of cost function:

$$\min_{u(\cdot)} J = \int_0^T L(u) dt. \quad (10)$$

We thus obtain a standard optimal control problem. To solve it, we construct the control Hamiltonian as follows [20]:

$$\mathcal{H} = \langle \Psi, [-iH, \rho] \rangle + L(u), \quad (11)$$

where Ψ is the costate matrix whose dynamics is given by

$$\dot{\Psi} = -\frac{\partial \mathcal{H}}{\partial \rho} = -[iH, \Psi]. \quad (12)$$

Let

$$\phi_l = \langle \Psi, [X_l, \rho] \rangle. \quad (13)$$

The control Hamiltonian can then be written as

$$\begin{aligned} \mathcal{H} &= -\left\langle \Psi, \left[\sum_{l=p+1}^K a_l X_l + \sum_{l=1}^p u_l X_l, \rho \right] \right\rangle + L(u) \\ &= -\sum_{l=p+1}^K a_l \phi_l - \sum_{l=1}^p u_l \phi_l + L(u). \end{aligned} \quad (14)$$

The optimality condition

$$\frac{d\mathcal{H}}{du} = 0 \quad (15)$$

yields that

$$\phi_l = \frac{dL}{du_l}, \quad (16)$$

for $l = 1, \dots, p$. Solving the algebraic equation Eq. (16), we can obtain the optimal controls as functions of ϕ_l . For the sake of completeness, we list all the optimality conditions as follows:

$$\begin{aligned} \dot{\rho} &= -[iH, \rho], \\ \dot{\Psi} &= -[iH, \Psi], \\ \rho_0 &= \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad \rho_T = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \\ \phi_l &= \frac{dL}{du_l}. \end{aligned} \quad (17)$$

This is a two-point boundary-value problem, which is often difficult to solve numerically. We consider to derive the dynamics for ϕ_l and then transform it into an optimization problem on finite dimensional space. Taking the derivative of ϕ_l :

$$\begin{aligned} \dot{\phi}_l &= \langle \dot{\Psi}, [X_l, \rho] \rangle + \langle \Psi, [X_l, \dot{\rho}] \rangle \\ &= \langle [-iH, \Psi], [X_l, \rho] \rangle + \langle \Psi, [X_l, [-iH, \rho]] \rangle \\ &= \langle \Psi, [iH, [X_l, \rho]] \rangle - \langle \Psi, [X_l, [iH, \rho]] \rangle \\ &= \langle \Psi, [[iH, X_l], \rho] \rangle, \end{aligned} \quad (18)$$

where the last equality follows from the Jacobi identity. For the Hamiltonian given by Eq. (7), we have

$$\begin{aligned} \dot{\phi}_l &= \left\langle \Psi, \left[\sum_{j=p+1}^K a_j X_j + \sum_{j=1}^p u_j X_j, X_l \right], \rho \right\rangle \\ &= \sum_{i=1}^K \left(\sum_{j=p+1}^K a_j C_{jl}^i + \sum_{j=1}^p u_j C_{jl}^i \right) \phi_i. \end{aligned} \quad (19)$$

Since the controls u_j can be determined from Eq. (16) as functions of ϕ , we can further rewrite Eq. (19) as a compact vector differential equation:

$$\dot{\phi} = F(\phi), \quad (20)$$

where $\phi = [\phi_1 \dots \phi_K]$. Note that the dynamics (19) is indeed a direct result from Lie-Poisson reduction theorem. See Chap. 13 of Ref. [19] and Ref. [21] for details.

Recalling that the structure constants C_{jl}^i are antisymmetric in all the indices, we obtain that

$$\begin{aligned} \frac{d}{dt} \|\phi\|^2 &= \frac{d}{dt} \left(\sum_{l=1}^K \phi_l^2 \right) = \sum_{l=1}^K 2\phi_l \dot{\phi}_l \\ &= 2 \sum_{l=1}^K \sum_{i=1}^K \phi_l \left(\sum_{j=p+1}^K a_j C_{jl}^i + \sum_{j=1}^p u_j C_{jl}^i \right) \phi_i = 0. \end{aligned}$$

Hence,

$$\|\phi\|^2 = \text{const}, \quad (21)$$

that is, $\|\phi\|$ is a conserved quantity along the optimal trajectory.

With the dynamics of ϕ in Eq. (19), we do not have to solve the difficult two-point boundary-value problem Eq. (17). Instead, we can assume an initial state of ϕ and solve the differential equation Eq. (19). If the resulting control fields u_l determined by solving Eq. (16) are optimal, they can transfer the density matrix from the initial condition to the desired terminal state; otherwise, we can calculate the fidelity of the actually achieved terminal state $\rho(T)$ as

$$J = \text{Tr } \rho_T \rho(T). \quad (22)$$

Now the state transfer problem can be cast into an optimization problem that maximizes the fidelity J in Eq. (22) by varying the initial condition of ϕ .

B. Numerical algorithm

We can apply a gradient algorithm to find the optimal initial condition $\phi^*(0)$ that maximizes the fidelity. To this end, we need to derive $dJ/d\phi_l(0)$, the gradient of the fidelity J with respect to the initial condition $\phi_l(0)$. Consider piecewise constant control functions. For a given time duration $[0, T]$, divide it into N equal intervals $\{[t_k, t_{k+1}]\}_{k=0}^{N-1}$ of length $\Delta t = t_{k+1} - t_k = T/N$, where $t_0 = 0$ and $t_N = T$. Within the interval $[t_k, t_{k+1}]$, the control field ϕ_l assumes a constant value $\phi_l(k)$.

By the chain rule, we have

$$\begin{aligned} \frac{dJ}{d\phi_l(0)} &= \sum_{k=0}^{N-1} \sum_{m=1}^p \frac{dJ}{du_m(k)} \frac{du_m(k)}{d\phi_l(0)} \\ &= \sum_{k=0}^{N-1} \sum_{m=1}^p \sum_{s=1}^K \frac{dJ}{du_m(k)} \frac{du_m(k)}{d\phi_s(k)} \frac{d\phi_s(k)}{d\phi_l(0)}. \end{aligned} \quad (23)$$

We thus need to derive the three differentials in the right hand side of Eq. (23). First consider $\frac{d u_m(k)}{d \phi_s(k)}$. From Eq. (16), we obtain

$$\frac{d}{d \phi_s} \left(\frac{dL}{d u_m} \right) = \frac{d}{d \phi_s} \phi_m = \delta_{ms}. \quad (24)$$

Because the running cost L is defined as a function of only the control fields u as in Eq. (10), $\frac{dL}{d u_m}$ is also a function of u only. Therefore, we can get $\frac{d u_m(k)}{d \phi_s(k)}$ by solving the algebraic equation Eq. (24). For example, when L is taken as a quadratic function $L = \frac{1}{2}(u_1^2 + u_2^2)$, it is immediate to obtain $\frac{d u_m}{d \phi_s} = \delta_{ms}$.

Next consider $\frac{d \phi_s(k)}{d \phi_l(0)}$. Recall that we have written the dynamics of ϕ in a compact vector differential equation (20). Differentiating both sides of Eq. (20) with respect to $\phi(0)$, we obtain

$$\frac{d}{d \phi(0)} \dot{\phi} = \frac{d}{d \phi(0)} F(\phi) = DF(\phi) \frac{d \phi}{d \phi(0)}, \quad (25)$$

where the Jacobian matrix $DF(\phi)$ is given by

$$DF(\phi) = \begin{bmatrix} \frac{\partial F_1}{\partial \phi_1} & \cdots & \frac{\partial F_1}{\partial \phi_K} \\ \vdots & & \vdots \\ \frac{\partial F_K}{\partial \phi_1} & \cdots & \frac{\partial F_K}{\partial \phi_K} \end{bmatrix}, \quad (26)$$

and

$$\frac{d \phi}{d \phi(0)} = \begin{bmatrix} \frac{\partial \phi_1}{\partial \phi_1(0)} & \cdots & \frac{\partial \phi_1}{\partial \phi_K(0)} \\ \vdots & & \vdots \\ \frac{\partial \phi_K}{\partial \phi_1(0)} & \cdots & \frac{\partial \phi_K}{\partial \phi_K(0)} \end{bmatrix}. \quad (27)$$

From Proposition 6.1 of Chapter 1 in Ref. [22], we have

$$\frac{d}{d \phi(0)} \dot{\phi} = \frac{d}{dt} \frac{d \phi}{d \phi(0)}, \quad (28)$$

that is, it is legitimate to change the order of the differentials with respect to t and $\phi(0)$. Combining Eq. (25) and Eq. (28), we get the differential equation satisfied by $\frac{d \phi}{d \phi(0)}$:

$$\frac{d}{dt} \frac{d \phi}{d \phi(0)} = DF(\phi) \frac{d \phi}{d \phi(0)}, \quad (29)$$

where the initial condition is given by

$$\left. \frac{d \phi}{d \phi(0)} \right|_{t=0} = I. \quad (30)$$

Solving the differential equation Eq. (29), we can get $\frac{d \phi_s(k)}{d \phi_l(0)}$.

Lastly derive $\frac{dJ}{d u_m(k)}$. From Eq. (7), we have

$$iH(k) = \sum_{l=p+1}^K a_l X_l + \sum_{l=1}^p u_l(k) X_l, \quad (31)$$

and $U_k = e^{-iH(k)\Delta t}$, where $k = 0, \dots, N-1$. Define

$$\begin{aligned} \rho_k &= U_{k-1} \cdots U_0 \rho_0 U_0^\dagger \cdots U_{k-1}^\dagger, \\ \Lambda_k &= U_k^\dagger \cdots U_{N-1}^\dagger \rho_T U_{N-1} \cdots U_k. \end{aligned}$$

Then $\rho_N = \rho(T)$, $\Lambda_N = \rho_T$, and

$$\begin{aligned} J &= \text{Tr} \rho_T \rho(T) = \text{Tr} \Lambda_N \rho_N = \text{Tr} \Lambda_{N-1} \rho_{N-1} \\ &= \cdots = \text{Tr} \Lambda_1 \rho_1 = \text{Tr} \Lambda_0 \rho_0. \end{aligned} \quad (32)$$

We need to derive the performance gradient with respect to control fields $u_m(k)$:

$$\begin{aligned} \frac{dJ}{d u_m(k)} &= \frac{d \text{Tr} \Lambda_{k+1} \rho_{k+1}}{d u_m(k)} = \frac{d \text{Tr} \Lambda_{k+1} U_k \rho_k U_k^\dagger}{d u_m(k)} \\ &= \text{Tr} \Lambda_{k+1} \left(\frac{d U_k}{d u_m(k)} \rho_k U_k^\dagger + U_k \rho_k \frac{d U_k^\dagger}{d u_m(k)} \right). \end{aligned} \quad (33)$$

From the following formula [23]

$$\left. \frac{d}{dv} e^{-i(H_a + v H_b)t} \right|_{v=0} = -i \int_0^t e^{-i H_a \tau} H_b e^{i H_a \tau} d\tau e^{-i H_a t}, \quad (34)$$

we have

$$\frac{d U_k}{d u_m(k)} = - \int_0^{\Delta t} e^{-i H(k) \tau} X_m e^{i H(k) \tau} d\tau U_k. \quad (35)$$

Substituting Eq. (35) into (33), we obtain

$$\begin{aligned} \frac{dJ}{d u_m(k)} &= \text{Tr} \Lambda_{k+1} \left(- \int_0^{\Delta t} e^{-i H(k) \tau} X_m e^{i H(k) \tau} d\tau \rho_{k+1} \right. \\ &\quad \left. + \rho_{k+1} \int_0^{\Delta t} e^{-i H(k) \tau} X_m e^{i H(k) \tau} d\tau \right) \\ &= \text{Tr} [\Lambda_{k+1}, \rho_{k+1}] \int_0^{\Delta t} e^{-i H(k) \tau} X_m e^{i H(k) \tau} d\tau. \end{aligned}$$

Since $H(k)$ is a Hermitian matrix, we can diagonalize it as

$$H(k) = T(k) \Gamma(k) T^\dagger(k), \quad (36)$$

where $T(k)$ is a unitary matrix and

$$\Gamma(k) = \text{diag}\{\gamma_1, \gamma_2, \gamma_3\}. \quad (37)$$

Therefore,

$$\begin{aligned} &\int_0^{\Delta t} e^{-i H(k) \tau} X_m e^{i H(k) \tau} d\tau \\ &= \int_0^{\Delta t} T(k) e^{-i \Gamma(k) \tau} T^\dagger(k) X_m T(k) e^{i \Gamma(k) \tau} T^\dagger(k) d\tau \\ &= T(k) \int_0^{\Delta t} (T^\dagger(k) X_m T(k)) \odot \Psi d\tau T^\dagger(k), \end{aligned} \quad (38)$$

where \odot denotes the Hadamard product, *i.e.*, element-wise product, of two matrices, and $\Psi_{ab} = e^{i(\gamma_b - \gamma_a)\tau}$. For $\gamma_a \neq \gamma_b$, we define

$$\Phi_{ab} = \int_0^{\Delta t} \Psi_{ab} d\tau = \frac{e^{i(\gamma_b - \gamma_a)\Delta t} - 1}{i(\gamma_b - \gamma_a)};$$

and for $\gamma_a = \gamma_b$, $\Phi_{ab} = \Delta t$. Therefore,

$$\begin{aligned} & \int_0^{\Delta t} e^{-iH(k)\tau} X_m e^{iH(k)\tau} d\tau \\ &= T(k) \left((T^\dagger(k) X_m T(k)) \odot \Phi \right) T^\dagger(k), \end{aligned}$$

and

$$\begin{aligned} \frac{dJ}{du_m(k)} &= \text{Tr}([\Lambda_{k+1}, \rho_{k+1}] T(k) \\ &\quad \cdot ((T^\dagger(k) X_m T(k)) \odot \Phi) T^\dagger(k)). \end{aligned} \quad (39)$$

We have now derived a closed form solution of $dJ/d\phi_l(0)$, the gradient of the fidelity J with respect to the initial condition $\phi_l(0)$. It is ready to implement gradient types of algorithms such as the gradient descent algorithm, the conjugate gradient method, and the BFGS method [24].

Note that Khaneja *et al* [25] developed the GRAPE algorithm to solve a similar problem. The difference between GRAPE and our algorithm is that GRAPE does not assume any correlation between neighboring control steps and the obtained control fields could thus be oscillatory. As a contrast, our algorithm optimizes over the initial condition of a differential equation and therefore the resulting control functions have correlation between neighboring steps.

We will then apply our algorithm to two physical systems, the triple quantum dot system discussed in Ref. [8] and the ionized donor chain discussed in Ref. [5]. The optimized control fields realizing the desired electron shuttling demonstrate the efficacy of our algorithm. For the ionized donor chain we further show that these optimized control fields can also provide a high degree of spin state transfer when the shuttled electron is coupled to the donor nuclei by the hyperfine interaction.

IV. TRIPLE QUANTUM DOT

We now investigate electron shuttling for the triple quantum dot system discussed in Ref. [8]. In this system, an electron beginning in the left dot of a three lateral quantum dot system is moved to the right dot. The relative energies of the left and right dots are controlled by external gate voltages. The Hamiltonian is given by

$$H = \begin{bmatrix} \mu_L(t) & J_1 & 0 \\ J_1 & 0 & J_2 \\ 0 & J_2 & \mu_R(t) \end{bmatrix}, \quad (40)$$

where the control fields are the on-site energies μ_L and μ_R , and J_1 and J_2 are the fixed coupling constants

between nearest neighboring dots. Using the basis in Eq. (1), we can rewrite the Hamiltonian (40) as

$$iH = J_1 X_1 + J_2 X_2 + \frac{\mu_L}{2} X_7 + \frac{\mu_L - 2\mu_R}{2\sqrt{3}} X_8 + \frac{\mu_L + \mu_R}{3} I_3 \quad (41)$$

Same as before, we consider the minimum energy cost function

$$\min J = \frac{1}{2} \int_0^T (\mu_L^2(\tau) + \mu_R^2(\tau)) d\tau.$$

The parameters in the Hamiltonian are

$$a_1 = J_1, \quad a_2 = J_2, \quad u_7 = \frac{\mu_L}{2}, \quad u_8 = \frac{\mu_L - 2\mu_R}{2\sqrt{3}}.$$

Hence

$$\mu_L = 2u_7, \quad \mu_R = u_7 - \sqrt{3}u_8,$$

and the running cost is

$$L(u) = \frac{\mu_L^2}{2} + \frac{\mu_R^2}{2} = 2u_7^2 + \frac{(u_7 - \sqrt{3}u_8)^2}{2}.$$

The optimality condition Eq. (16) becomes

$$\phi_7 = 5u_7 - \sqrt{3}u_8, \quad \phi_8 = 3u_8 - \sqrt{3}u_7,$$

which yields that

$$u_7 = \frac{\sqrt{3}\phi_7 + \phi_8}{4\sqrt{3}}, \quad u_8 = \frac{\sqrt{3}\phi_7 + 5\phi_8}{12},$$

and then

$$\mu_L = \frac{\sqrt{3}\phi_7 + \phi_8}{2\sqrt{3}}, \quad \mu_R = -\frac{\phi_8}{\sqrt{3}}.$$

We can now obtain the dynamics of ϕ as

$$\begin{aligned} \dot{\phi}_1 &= J_2 \phi_3 - \phi_4 \phi_7 / 2 - \sqrt{3} / 6 \phi_4 \phi_8 \\ \dot{\phi}_2 &= -J_1 \phi_3 - \phi_5 \phi_8 / \sqrt{3} \\ \dot{\phi}_3 &= -J_2 \phi_1 + J_1 \phi_2 + \phi_6 \phi_7 / 2 + \sqrt{3} / 2 \phi_6 \phi_8 \\ \dot{\phi}_4 &= \phi_1 \phi_7 / 2 + \sqrt{3} / 6 \phi_1 \phi_8 - J_2 \phi_6 - 2J_1 \phi_7 \\ \dot{\phi}_5 &= \phi_2 \phi_8 / \sqrt{3} + J_1 \phi_6 + J_2 \phi_7 - \sqrt{3} J_2 \phi_8 \\ \dot{\phi}_6 &= -\phi_3 \phi_7 / 2 - \sqrt{3} / 2 \phi_3 \phi_8 + J_2 \phi_4 - J_1 \phi_5 \\ \dot{\phi}_7 &= 2J_1 \phi_4 - J_2 \phi_5 \\ \dot{\phi}_8 &= \sqrt{3} J_2 \phi_5 \end{aligned} \quad (42)$$

The gradient of the fidelity J with respect to $\phi_l(0)$ can be written as

$$\begin{aligned} \frac{dJ}{d\phi_l(0)} &= \sum_{k=0}^{N-1} \sum_{m=1}^p \sum_{s=1}^K \frac{dJ}{du_m(k)} \frac{du_m(k)}{d\phi_s(k)} \frac{d\phi_s(k)}{d\phi_l(0)} \\ &= \sum_{k=0}^{N-1} \left(\frac{1}{4} \frac{dJ}{du_7(k)} \frac{d\phi_7(k)}{d\phi_l(0)} + \frac{1}{4\sqrt{3}} \frac{dJ}{du_7(k)} \frac{d\phi_8(k)}{d\phi_l(0)} \right. \\ &\quad \left. + \frac{1}{4\sqrt{3}} \frac{dJ}{du_8(k)} \frac{d\phi_7(k)}{d\phi_l(0)} + \frac{5}{12} \frac{dJ}{du_8(k)} \frac{d\phi_8(k)}{d\phi_l(0)} \right). \end{aligned}$$

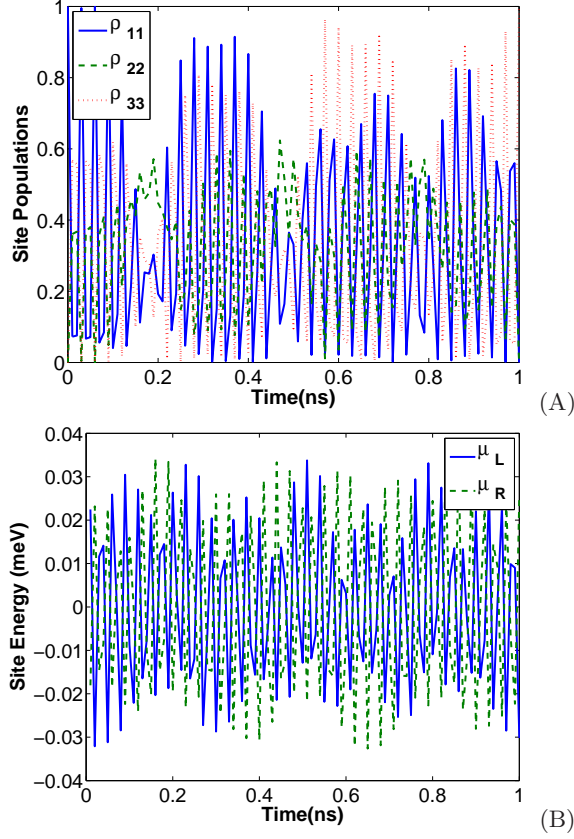


FIG. 1: (A) State transfer. Blue solid: ρ_{11} ; Green dashed: ρ_{22} ; Red dotted: ρ_{33} . J_1 and J_2 were set to -0.1 meV. (B) Control functions. Blue solid: μ_L ; Green dashed: μ_R . The pulses are given for $N = 100$ segments. (See electronic version for color plots).

The Jacobian matrix $DF(\phi)$ is

$$\begin{bmatrix} 0 & 0 & J_2 & -\frac{\phi_7}{2} & 0 & 0 & -\frac{\phi_4}{2} & -\frac{\sqrt{3}\phi_4}{6} \\ 0 & 0 & -J_1 & 0 & -\frac{\phi_8}{\sqrt{3}} & 0 & 0 & -\frac{\phi_5}{\sqrt{3}} \\ -J_2 & J_1 & 0 & 0 & 0 & \frac{\sqrt{3}\phi_8}{2} & \frac{\phi_6}{2} & \frac{\sqrt{3}\phi_6}{2} \\ \frac{\sqrt{3}\phi_8}{6} & 0 & 0 & 0 & 0 & -J_2 & \frac{\phi_1}{2} & \frac{\sqrt{3}\phi_1}{6} \\ +\frac{\phi_7}{2} & 0 & 0 & 0 & 0 & -J_2 & -2J_1 & \frac{\phi_2}{\sqrt{3}} \\ 0 & \frac{\phi_8}{\sqrt{3}} & 0 & 0 & 0 & J_1 & J_2 & -\frac{\phi_3}{\sqrt{3}} \\ 0 & 0 & -\frac{\sqrt{3}\phi_8}{2} & J_2 & -J_1 & 0 & -\frac{\phi_3}{2} & -\frac{\sqrt{3}\phi_3}{2} \\ 0 & 0 & 0 & 2J_1 & -J_2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \sqrt{3}J_2 & 0 & 0 & 0 \end{bmatrix}.$$

In Fig. 1, the state transfer in $N = 100$ segments is plotted for J_1 and J_2 set to -0.1 meV and a transfer time of 1 ns.

V. IONIZED DONOR CHAIN

In this section we apply our control algorithm to the ionized donor chain studied in Ref. [5]. The system consists of three singly ionized phosphorus donors in silicon, and one electron shared in the system. The electron begins on the first phosphorus, site 1, and the pulses are designed to move this electron to site 3. The Hamiltonian is given by (setting $\hbar = 1$):

$$H = \begin{bmatrix} 0 & -\Omega_{12}(t) & 0 \\ -\Omega_{12}(t) & \Delta & -\Omega_{23}(t) \\ 0 & -\Omega_{23}(t) & 0 \end{bmatrix}. \quad (43)$$

Here the control terms are Ω_{12} and Ω_{23} , which are the coherent tunneling rate between adjacent dopants. Under the basis in Eq. (1), this Hamiltonian can be written as

$$iH = -\Omega_{12}X_1 - \Omega_{23}X_2 - \frac{\Delta}{2}X_7 + \frac{\Delta}{2\sqrt{3}}X_8 + \frac{\Delta}{3}I_3. \quad (44)$$

We can drop the term $\frac{\Delta}{3}I_3$ as it commutes with all the other terms and thus contributes only a global phase. Consider the following minimum energy cost function

$$\min J = \frac{1}{2} \int_0^T (\Omega_{12}^2(\tau) + \Omega_{23}^2(\tau)) d\tau$$

with the initial and terminal states given in Eqs. (8)-(9). Following the procedure in Sec. III, we have the parameters in the Hamiltonian are

$$u_1 = -\Omega_{12}, \quad u_2 = -\Omega_{23}, \quad a_7 = -\frac{\Delta}{2}, \quad a_8 = \frac{\Delta}{2\sqrt{3}},$$

and the running cost is

$$L(u) = \frac{u_1^2}{2} + \frac{u_2^2}{2}.$$

The optimality condition Eq. (16) yields that

$$\phi_1 = u_1, \quad \phi_2 = u_2.$$

Hence the optimal controls are given by

$$\Omega_{12} = -\phi_1, \quad \Omega_{23} = -\phi_2. \quad (45)$$

For the Hamiltonian (44), the dynamics of ϕ in Eq. (19) becomes

$$\dot{\phi}_l = \sum_{i=1}^K \left(\phi_1 C_{1l}^i + \phi_2 C_{2l}^i - \frac{\Delta}{2} C_{7l}^i + \frac{\Delta}{2\sqrt{3}} C_{8l}^i \right) \phi_i, \quad (46)$$

Substituting the values of structure constants C_{ij}^k in Eq. (4) into Eq. (46), we obtain the complete dynam-

ics of ϕ :

$$\begin{aligned}
\dot{\phi}_1 &= \phi_2\phi_3 + \Delta\phi_4 \\
\dot{\phi}_2 &= -\phi_1\phi_3 - \Delta\phi_5 \\
\dot{\phi}_3 &= 0 \\
\dot{\phi}_4 &= -\Delta\phi_1 - \phi_2\phi_6 - 2\phi_1\phi_7 \\
\dot{\phi}_5 &= \Delta\phi_2 + \phi_1\phi_6 + \phi_2\phi_7 - \sqrt{3}\phi_2\phi_8 \\
\dot{\phi}_6 &= \phi_2\phi_4 - \phi_1\phi_5 \\
\dot{\phi}_7 &= 2\phi_1\phi_4 - \phi_2\phi_5 \\
\dot{\phi}_8 &= \sqrt{3}\phi_2\phi_5.
\end{aligned} \tag{47}$$

To implement the numerical algorithm, it is easy to get that

$$\frac{dJ}{d\phi_i(0)} = \sum_{k=0}^{N-1} \left(\frac{dJ}{du_1(k)} \frac{d\phi_1(k)}{d\phi_i(0)} + \frac{dJ}{du_2(k)} \frac{d\phi_2(k)}{d\phi_i(0)} \right). \tag{48}$$

The Jacobian matrix $DF(\phi)$ can be derived from Eq. (47) as

$$\begin{bmatrix}
0 & \phi_3 & \phi_2 & \Delta & 0 & 0 & 0 & 0 \\
-\phi_3 & 0 & -\phi_1 & 0 & -\Delta & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
-\Delta & -\phi_6 & 0 & 0 & 0 & -\phi_2 & -2\phi_1 & 0 \\
\phi_6 & \Delta + \phi_7 & 0 & 0 & 0 & \phi_1 & \phi_2 & -\sqrt{3}\phi_2 \\
-\phi_5 & -\sqrt{3}\phi_8 & 0 & 0 & 0 & \phi_1 & \phi_2 & -\sqrt{3}\phi_2 \\
-\phi_5 & \phi_4 & 0 & \phi_2 & -\phi_1 & 0 & 0 & 0 \\
2\phi_4 & -\phi_5 & 0 & 2\phi_1 & -\phi_2 & 0 & 0 & 0 \\
0 & \sqrt{3}\phi_5 & 0 & 0 & \sqrt{3}\phi_2 & 0 & 0 & 0
\end{bmatrix}.$$

For the particular Hamiltonian (44), we can derive an analytic solution for the decomposition in Eq. (36). The eigenvalues of $H(k)$ are

$$\gamma_1 = -\frac{\Delta}{3}, \quad \gamma_2 = \frac{\Delta + 3g_1}{6}, \quad \gamma_3 = \frac{\Delta - 3g_1}{6},$$

and the unitary matrix $T(k)$ is

$$\begin{bmatrix}
-\Omega_{23}/g_2 & \Omega_{12}/\sqrt{g_1(g_1 + \Delta)/2} & \Omega_{12}/\sqrt{g_1(g_1 - \Delta)/2} \\
0 & -\sqrt{(g_1 + \Delta)/(2g_1)} & \sqrt{(g_1 - \Delta)/(2g_1)} \\
\Omega_{12}/g_2 & \Omega_{23}/\sqrt{g_1(g_1 + \Delta)/2} & \Omega_{23}/\sqrt{g_1(g_1 - \Delta)/2}
\end{bmatrix},$$

where $g_1 = \sqrt{\Delta^2 + 4\Omega_{23}^2 + 4\Omega_{12}^2}$ and $g_2 = \sqrt{\Omega_{23}^2 + \Omega_{12}^2}$.

In Fig. 2, the optimized pulses in $N = 100$ segments are shown for $\Delta = 2.7$ meV, for a transfer time of 1 ns. This is in line with the values calculated using tight binding theory [7]. In Fig. 2(A), the populations of each site are shown as a function of time, the populations is fully transferred from the first to the third site, and the middle site maintains a relatively low populations throughout.

Since one of the main qubits of interest is phosphorus-doped silicon, in which quantum information is stored in the spin of the electrons and nuclei, we also used these pulses to attempt to transfer a hyperfine spin state along with spatially transferring the electron. For these calculations, a hyperfine interaction with a splitting of 117.5

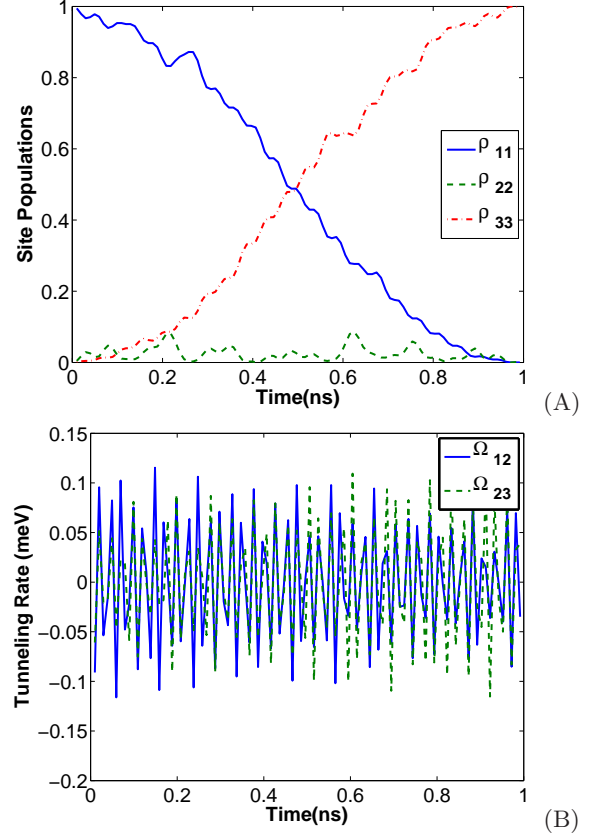


FIG. 2: (A) State transfer. Blue solid: ρ_{11} ; Green dashed: ρ_{22} ; Red dotted: ρ_{33} . The value of Δ was set to 2.7 meV. (B) Control functions. Blue solid: Ω_{12} ; Green dashed: Ω_{23} . The pulses are given for $N = 100$ segments. (See electronic version for color plots).

MHz was used [26]. The results are shown in Fig. 3 for no external magnetic field (A) and a field of 500 G (B). The spins of the nuclei at sites 2 and 3 are initialized into the \uparrow state, while on site 1 the electron-nuclear system is initialized into one of four hyperfine eigenstates. The distance measure (D) shown in Fig. 3 is a measure of the transfer of this hyperfine state,

$$D = 1 - \|\rho_T - \rho_{hf}\|_2, \tag{49}$$

where ρ_{hf} is the density matrix for one of the hyperfine pure states, and ρ_T is the reduced density matrix of the site 3 nuclear and electron spin at the end of the spatial transfer. The norm used in Eq. (49) is the induced 2-norm of the difference matrix, also known as the spectral norm, which is the maximum singular value of the matrix [27]. We have also calculated the fidelity [28, 29], the trace distance [28], and the Frobenius norm of the difference matrix [27], and while all norms show a similar picture regarding which states are transferred, the measure D has the pictorial advantage of following the population on the third site when full transfer is occurring as well as remaining zero when the fidelity is zero,

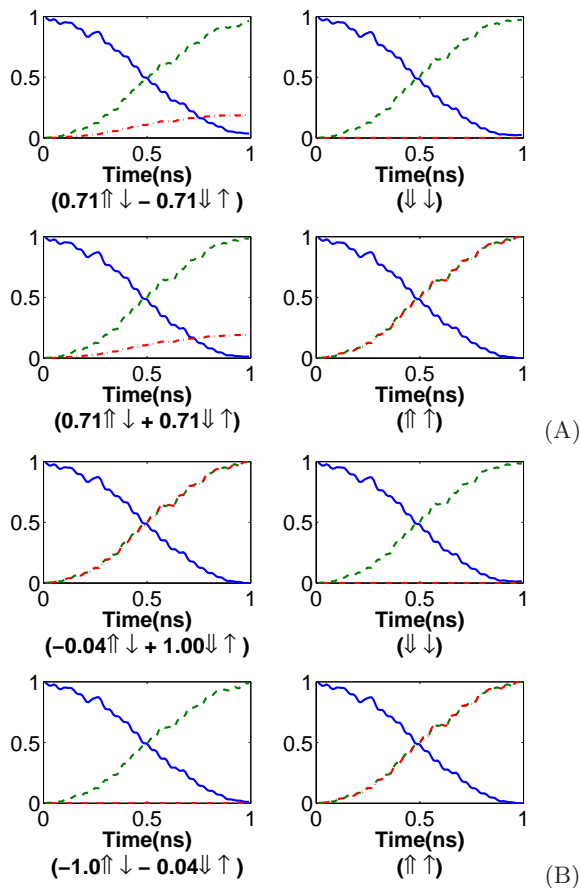


FIG. 3: (A) Transfer of hyperfine eigenstates are attempted using the pulses in Fig. 2. The population of sites 1 (solid blue) and 3 (dashed green) are shown as well as the measure D of the hyperfine state transfer (Eq. (49)) at site 3 (dotted red). (B) The same as (A), but with the addition of a magnetic field (500 G). The hyperfine states which align the nuclear spin with the magnetic field can be transferred, while the spin flipped states are energetically forbidden. (See electronic version for color plots).

unlike the Frobenius norm. At all magnetic fields, the $|\uparrow\uparrow\rangle$ state can be transferred completely from site 1 to site 3, because with all of the nuclear spins up the electrons remain in the hyperfine eigenstate no matter which spatial site it is on. Conversely, the hyperfine state $|\downarrow\downarrow\rangle$ cannot be transferred, because this would require flipping the spins of the nuclei on sites 2 and 3, which is not allowed energetically. The electrons which start in this state can be transferred spatially, however. Calculations have shown that for larger hyperfine constants the spatial transfer of the electron can be reduced in the presence of the hyperfine interaction. For the linear combinations of $|\uparrow\downarrow\rangle$ and $|\downarrow\uparrow\rangle$, partial transfers can be accomplished

corresponding to the contribution from the part of the linear combination which has the nuclear spin up. This can be seen because as the magnetic field is turned on (Fig. 3(B)) and the linear combinations goes from equal to being largely one component or the other, the transfer of the component which is mostly nuclear spin up can be achieved while transferring the mostly nuclear spin down cannot. It should be noted that in the case of a 500 G magnetic field, two hyperfine states can be transferred spatially, suggesting their potential use as a mobile qubit.

VI. CONCLUSION

In this paper we have formulated a general problem in solid-state electron shuttling as a state transfer problem in optimal control theory. We derived the underlying dynamical equations that govern the time evolution of optimal control fields. This leads to an efficient numerical algorithm with a small number of optimizing variables. We demonstrate the efficiency of our algorithm by two physical examples.

First, we determined the control pulses for state transfer between left and right quantum dots in a triple quantum dot system. Since hyperfine interactions in lateral quantum dots can be small, such spatial transfer allows the ability to transmit quantum information and possibly use this ability to couple qubits. Second, we looked at the system of an ionized phosphorus donor chain in silicon. We again determined optimal control pulses for spatial transfer, and then we looked at the transfer of a spin qubit using these pulses with hyperfine interactions considered. In the 500 G magnetic field case, two hyperfine states of the electron and nucleus can be transferred in such a donor chain. As the field is decreased, however, only one of four hyperfine states can be spatially transferred. Therefore, in order to transfer spin quantum information in a donor chain in a low-field environment, control pulses which take the spin interactions into account are desired.

Acknowledgments

JZ thanks the financial support from the Innovation Program of Shanghai Municipal Education Commission under Grant No. 11ZZ20, Shanghai Pujiang Program under Grant No. 11PJ1405800, NSFC under Grant No. 61174086, and State Key Lab of Advanced Optical Communication Systems and Networks, SJTU, China. XD thanks the University of California-Berkeley College of Chemistry Summer Research Stipend. We thank NSA (Grant No. MOD713106A) for financial support.

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